Polder maps: Improving OMIT maps for ligand building and validation

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In macromolecular crystallography, electron density maps are used to build and validate models. In particular, OMIT maps [1] are a common tool to verify the presence of ligands. The simplest way to compute an OMIT map is to exclude the ligand from the model, update the structure factors and compute a residual map. If the ligand is present in the crystal structure, it is expected that the electron density of the ligand will appear as positive features in the OMIT map. However, this is complicated by the flat bulk-solvent model [2], which postulates constant electron density in the areas of the unit cell that are not occupied by the atomic model. Therefore, if atoms are removed from the model, the region where they were modeled will be filled with bulk-solvent, and if the density arising from the omitted atoms is weak, then the bulk-solvent model may obscure it further.

A possible solution to this problem is to prevent bulk-solvent from entering the OMIT regions, which may improve the interpretative power of residual maps. This approach is called polder (OMIT) map [3] and the tool is implemented and available in the software suite Phenix [4]. Polder OMIT maps can be particularly useful for displaying weak densities of ligands (Fig. 1). Several examples are presented where polder OMIT maps show clearer features than conventional OMIT maps.

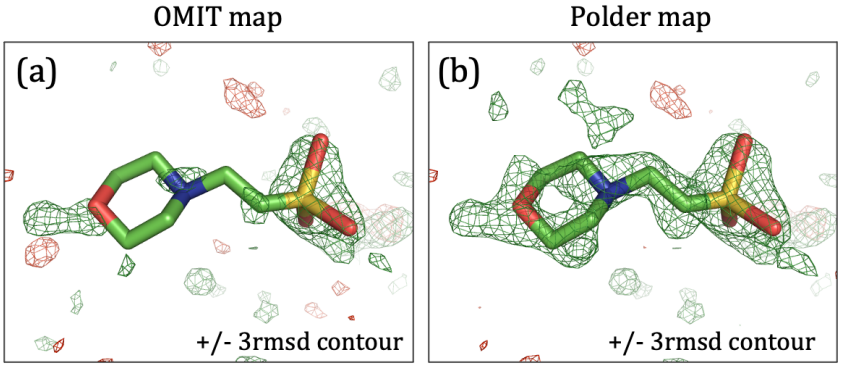

Fig. 1: OMIT map (a) and polder map of a MES solvent molecule in model 1ABA (1.45 Å resolution).

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